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$%^STN;HighlightOn= ***;HighlightOff=*** ;
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Welcome to STN International! Enter x:X
LOGINID: SSPTAPEZ1617
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2
                     Welcome to STN International
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NEWS 2 APR 04 STN AnaVist, Version 1, to be discontinued
NEWS 3 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new
                 predefined hit display formats
      4 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS
         APR 28 IMSRESEARCH reloaded with enhancements
NEWS 5
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family
                 searching
NEWS
      7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology
                 sequence search option
NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character
                 patent numbers for U.S. applications
NEWS 11 JUN 19 CAS REGISTRY includes selected substances from
                 web-based collections
NEWS 12 JUN 25 CA/CAplus and USPAT databases updated with IPC
                 reclassification data
NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S.
                 patent records
NEWS 14
         JUN 30
                 EMBASE, EMBAL, and LEMBASE updated with additional
                 options to display authors and affiliated
                 organizations
NEWS 15
         JUN 30 STN on the Web enhanced with new STN AnaVist
                 Assistant and BLAST plug-in
NEWS 16 JUN 30 STN AnaVist enhanced with database content from EPFULL
NEWS 17 JUL 28 CA/Caplus patent coverage enhanced
NEWS 18 JUL 28 EPFULL enhanced with additional legal status
                 information from the epoline Register
NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20 JUL 28 STN Viewer performance improved
NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts
                 page images from 1967-1998
NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS 24 AUG 15 CAplus currency for Korean patents enhanced
NEWS 25 AUG 25 CA/CAplus, CASREACT, and IFI and USPAT databases
                 enhanced for more flexible patent number searching
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NEWS 26 AUG 27 CAS definition of basic patents expanded to ensure

comprehensive access to substance and sequence

## information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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FILE 'HOME' ENTERED AT 10:37:38 ON 08 SEP 2008

=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10542351.str

L1 STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1 STR
/ Structure 1 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 10:38:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 105 TO ITERATE

100.0% PROCESSED 105 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 1486 TO 2714

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss ful

FULL SEARCH INITIATED 10:38:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2279 TO ITERATE

100.0% PROCESSED 2279 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

L3 2 SEA SSS FUL L1

=> file cap

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
178.36
178.57

FILE 'CAPLUS' ENTERED AT 10:38:26 ON 08 SEP 2008
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FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 13

L4 2 L3

=> d 14 1-2 ibib abs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:633527 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:174078

TITLE: Preparation of thienylpyridinecarbonitriles as

bacterial enoyl-ACP reductase (FabI) inhibitors.

INVENTOR(S): Moir, Donald T.; Xiang, Yibin; Arvanites, Anthony C.;

Ali, Syed Masarrat; Geng, Bolin; Ashwell, Mark A.;

Orgueira, Hernan Antonio

PATENT ASSIGNEE(S): Genome Therapeutics Corporation, USA; Arqule

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND		DATE		APPLICATION NO.						DATE				
WO 2004064	A1 20040805				WO 2	004-	US13	20040116							
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Ci	, co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
GI	GH,	GM,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,
LI	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ		
US 2007002	A1		2007	0201		US 2	006-	5423	20060807						
PRIORITY APPLN						US 2	003-	4414	11P		P 2	0030	117		
								WO 2	004-	US13	27		W 2	0040	116

OTHER SOURCE(S): MARPAT 141:174078

GΙ

/ Structure 2 in file .gra /

Title compds. I [R1, R2 = (un)substituted monocyclic aryl, heteroaryl; Y = X1-X2; X1 = bond, (un)substituted alkylene; X2 = aryl, heteroaryl, cycloaliph., etc.] and their pharmaceutically acceptable salts were prepd. For example, condensation-annulation of 1,3-di-2-thienyl-2-propen-1-one and 2-cyanoethanethioamide, followed by 4-(bromomethyl)benzoic acid S-alkylation of the resulting thioxopyridinecarbonitrile (no data provided), afforded claimed thienylpyridinecarbonitrile II. In methicillin-resistant Staphylococcus aureus minimal inhibitory concn. (MIC) assays, 14-examples of compds. I exhibited MIC values ranging from 0.75->64 .mu.g/mL, e.g., the MIC value of thienylpyridinecarbonitrile II

was 4 .mu.g/mL. Compds. I are claimed useful for the. Of note, compds. I are proposed to inhibit bacterial enoyl-ACP reductase (FabI), a NADH-dependent enoyl [acyl carrier protein] reductase enzyme in the fatty acid biosynthesis pathway.

IT \*\*\*340808-61-9P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of thienylpyridinecarbonitriles as bacterial enoyl-ACP reductase (FabI) inhibitors.)

RN 340808-61-9 CAPLUS

CN Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA INDEX NAME)

/ Structure 3 in file .gra /

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:374624 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:239652

TITLE: Identification and characterization of inhibitors of

bacterial enoyl-acyl carrier protein reductase

AUTHOR(S): Ling, Losee L.; Xian, Jun; Ali, Syed; Geng, Bolin;

Fan, Jun; Mills, Debra M.; Arvanites, Anthony C.;
Orqueira, Hernan; Ashwell, Mark A.; Carmel, Gilles;

Xiang, Yibin; Moir, Donald T.

CORPORATE SOURCE: Genome Therapeutics Corporation, Waltham, MA, 02453,

USA

SOURCE: Antimicrobial Agents and Chemotherapy (2004), 48(5),

1541-1547

CODEN: AMACCQ; ISSN: 0066-4804 American Society for Microbiology

DOCUMENT TYPE: Journal LANGUAGE: English

PUBLISHER:

Bacterial enoyl-acyl carrier protein reductase (ENR) catalyzes an essential step in fatty acid biosynthesis. ENR is an attractive target for narrow-spectrum antibacterial drug discovery because of its essential role in metab. and its sequence conservation across many bacterial species. In addn., the bacterial ENR sequence and structural organization are distinctly different from those of mammalian fatty acid biosynthesis enzymes. High-throughput screening to identify inhibitors of Escherichia coli ENR yielded four structurally distinct classes of hits. members of one of these, the 2-(alkylthio)-4,6-diphenylpyridine-3carbonitriles ("thiopyridines"), inhibited both purified ENR (50% inhibitory concn. [IC50] = 3-25 .mu.M) and the growth of Staphylococcus aureus and Bacillus subtilis (MIC =  $1-64 \cdot mu.g/mL$ ). The effect on cell growth is due in part to inhibition of fatty acid biosynthesis as judged by inhibition of incorporation of [14C]acetate into fatty acids and by the increased sensitivity of cells that underexpress an ENR-encoding gene (4-8-fold MIC shift). Synthesis of a variety of compds. in this chem. series revealed a correlation between IC50 and MIC, and the results provided initial structure-activity relationships. Preliminary structure-activity relationships, potency on purified ENR, and activity on bacterial cells indicate that members of the thiopyridine chem. series are

effective fatty acid biosynthesis inhibitors suitable for further antibacterial development.

RN 340808-61-9 CAPLUS

CN Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA INDEX NAME)

/ Structure 4 in file .gra /

RN 750595-50-7 CAPLUS

CN Benzoic acid, 4-[1-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]- (CA INDEX NAME)

/ Structure 5 in file .gra /

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 11.86 190.43

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NEWS 4 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family
                searching
     7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology
NEWS
                sequence search option
NEWS 8
       JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character
                patent numbers for U.S. applications
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                web-based collections
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                reclassification data
NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S.
                patent records
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                options to display authors and affiliated
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       JUN 30 STN on the Web enhanced with new STN AnaVist
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NEWS 18 JUL 28 EPFULL enhanced with additional legal status
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NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
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                page images from 1967-1998
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                enhanced for more flexible patent number searching
NEWS 26 AUG 27
                CAS definition of basic patents expanded to ensure
                comprehensive access to substance and sequence
                information
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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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E FILE TOTAL ENTRY SESSION 0.42 0.42

TOTAL

SINCE FILE

FULL ESTIMATED COST

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http://www.cas.org/support/stngen/stndoc/properties.html

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STRUCTURE UPLOADED L1

=> d 11

L1 HAS NO ANSWERS

L1 STR

/ Structure 6 in file .gra /

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=> s 11

SAMPLE SEARCH INITIATED 10:52:13 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -42 TO ITERATE

42 ITERATIONS 100.0% PROCESSED 27 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\* PROJECTED ITERATIONS: 452 TO 1228 229 TO PROJECTED ANSWERS: 851 => s 11 sss ful

FULL SEARCH INITIATED 10:52:21 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 554 TO ITERATE

100.0% PROCESSED 554 ITERATIONS

SEARCH TIME: 00.00.01

L3 342 SEA SSS FUL L1

=> file cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

342 ANSWERS

FULL ESTIMATED COST 178.36 178.78

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FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

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http://www.cas.org/legal/infopolicy.html

=> s 13

L4 5 L3

=> d 14 1-5 ibib abs hitstr

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1016002 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 142:6311

TITLE: A preparation of benzamide derivatives, useful as

glyoxalase inhibitors

INVENTOR(S): Ashton, Mark; Davidson, Alan; Thomas, Russell;

Whittaker, Mark

PATENT ASSIGNEE(S): Chroma Therapeutics Limited, UK

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION: \_\_\_\_\_

Pž	PATENT NO.					KIND DATE					LICAT									
W(	2004	2004101506					2004	1125												
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	, EC,	EE,	EG,	ES,	FΙ,	GB,	GD,			
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	, JP,	KE,	KG,	KP,	KR,	KΖ,	LC,			
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG	, MK,	MN,	MW,	MX,	MΖ,	NA,	NI,			
		NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU	, SC,	SD,	SE,	SG,	SK,	SL,	SY,			
		ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	, UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
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		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	, GA,	GN,	GQ,	GW,	ML,	MR,	NE,			
		SN,	TD,	ΤG																
Αl	AU 2004238625									AU 2004-238625										
	CA 2525438							CA 2004-2525438												
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	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	, IT,	LI,	LU,	NL,	SE,	MC,	PT,			
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	US 20070015799				A1		2007	0118			2005-					0051				
PRIORI:	PRIORITY APPLN. INFO.:										2003-									
										WO 2	2004-	GB21	01	,	W 2	0040	514			
OTHER :	SOURCE		MAR:	PAT	142:	6311														

GΙ

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/ Structure 7 in file .gra /
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The invention relates to a prepn. of benzamide derivs. of formula I AΒ [wherein: X is N or CH; R1 is H, CN, halogen, NH2, or S-alkyl, etc.; R2 is H, CF3, (un)substituted aryl, cycloalkyl, or heterocyclyl, etc.; R3 is the same as R2 excluding CF3; R4 is H, (un)substituted aryl or heterocyclyl; R5 is H, (un) substituted alkyl, aryl, or alkylene-aryl; L1 is (un) substituted alkylene, arylene, or alkylene-arylene, etc.; L2 is a single bond, (un)substituted alkylene, or C(0)-alkylene, etc.; L3 and L4 are independently selected from a single bond, (un) substituted alkylene, or alkylene-NHN(OH)C(O)-arylene, etc.], useful as glyoxalase inhibitors. For instance, benzamide deriv. II (R6 = OH; 80% proliferation inhibition in HL60s, IC50 = 8.3 .mu.M) was prepd. via hydrolysis of N-(benzoyloxy) benzamide II [R6 = OC(0)Ph] with a yield of 41%. ΙT

\*\*\*354555-67-2P\*\*\*

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzamide derivs. useful as glyoxalase inhibitors)

RN 354555-67-2 CAPLUS

Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-(CA INDEX NAME)

/ Structure 8 in file .gra /

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:633527 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:174078

TITLE: Preparation of thienylpyridinecarbonitriles as bacterial enoyl-ACP reductase (FabI) inhibitors.

INVENTOR(S): Moir, Donald T.; Xiang, Yibin; Arvanites, Anthony C.;

Ali, Syed Masarrat; Geng, Bolin; Ashwell, Mark A.;

Orgueira, Hernan Antonio

PATENT ASSIGNEE(S): Genome Therapeutics Corporation, USA; Arqule

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND		DATE			APPL	ICAT	ION 1		DATE			
WO 2004064837					A1 20040805					004-1	11013	20040116					
WO	WU 200400483/			AI		2004	0005		WO Z	004-	0513.	20040116					
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		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,
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US 20070027190					A1		2007	0201		US 2	006-	5423.	20060807				
PRIORITY APPLN. INFO.:										US 2	003-	4414	11P		P 2	0030	117
										WO 2	004-	US13:	27	1	W 2	0040	116

OTHER SOURCE(S): MARPAT 141:174078

GΙ

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/ Structure 9 in file .gra /
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AB Title compds. I [R1, R2 = (un) substituted monocyclic aryl, heteroaryl; Y = X1-X2; X1 = bond, (un) substituted alkylene; X2 = aryl, heteroaryl, cycloaliph., etc.] and their pharmaceutically acceptable salts were prepd. For example, condensation-annulation of 1,3-di-2-thienyl-2-propen-1-one and 2-cyanoethanethioamide, followed by 4-(bromomethyl) benzoic acid S-alkylation of the resulting thioxopyridinecarbonitrile (no data provided), afforded claimed thienylpyridinecarbonitrile II. In methicillin-resistant Staphylococcus aureus minimal inhibitory concn. (MIC) assays, 14-examples of compds. I exhibited MIC values ranging from 0.75->64 .mu.g/mL, e.g., the MIC value of thienylpyridinecarbonitrile II was 4 .mu.g/mL. Compds. I are claimed useful for the. Of note, compds. I are proposed to inhibit bacterial enoyl-ACP reductase (FabI), a NADH-dependent enoyl [acyl carrier protein] reductase enzyme in the fatty acid biosynthesis pathway.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

```
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of thienylpyridinecarbonitriles as bacterial enoyl-ACP
        reductase (FabI) inhibitors.)
RN
     296797-06-3 CAPLUS
CN
    Acetamide, N-[3-(acetylamino)phenyl]-2-[(3-cyano-4,6-di-2-thienyl-2-
    pyridinyl)thio]- (CA INDEX NAME)
/ Structure 10 in file .gra /
RN
     340808-61-9 CAPLUS
    Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
     INDEX NAME)
/ Structure 11 in file .gra /
     354555-67-2 CAPLUS
RN
CN
     Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-
     (CA INDEX NAME)
/ Structure 12 in file .gra /
RN
    733052-04-5 CAPLUS
CN
     Benzoic acid, 4-[2-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
     (CA INDEX NAME)
/ Structure 13 in file .gra /
     733052-05-6 CAPLUS
RN
CN
     3-Pyridinecarbonitrile, 2-[(1-phenylethyl)thio]-4,6-di-2-thienyl- (CA
     INDEX NAME)
/ Structure 14 in file .gra /
RN
     733052-06-7 CAPLUS
     Benzoic acid, 3-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
     INDEX NAME)
/ Structure 15 in file .gra /
     733052-07-8 CAPLUS
RN
     Benzeneacetic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]-
       (CA INDEX NAME)
/ Structure 16 in file .gra /
RN
     733052-09-0 CAPLUS
CN
     Propanoic acid, 3-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]- (CA INDEX
    NAME)
```

```
/ Structure 17 in file .gra /
       ***243987-05-5P***
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of thienylpyridinecarbonitriles as bacterial enoyl-ACP
        reductase (FabI) inhibitors.)
     243987-05-5 CAPLUS
RN
CN
     3-Pyridinecarbonitrile, 1,2-dihydro-4,6-di-2-thienyl-2-thioxo- (CA INDEX
     NAME)
/ Structure 18 in file .gra /
REFERENCE COUNT:
                         3
                               THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2004:374624 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         141:239652
                         Identification and characterization of inhibitors of
TITLE:
                         bacterial enoyl-acyl carrier protein reductase
                         Ling, Losee L.; Xian, Jun; Ali, Syed; Geng, Bolin;
AUTHOR(S):
                         Fan, Jun; Mills, Debra M.; Arvanites, Anthony C.;
                         Orgueira, Hernan; Ashwell, Mark A.; Carmel, Gilles;
                         Xiang, Yibin; Moir, Donald T.
CORPORATE SOURCE:
                         Genome Therapeutics Corporation, Waltham, MA, 02453,
                         USA
SOURCE:
                         Antimicrobial Agents and Chemotherapy (2004), 48(5),
                         1541-1547
                         CODEN: AMACCQ; ISSN: 0066-4804
PUBLISHER:
                         American Society for Microbiology
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Bacterial enoyl-acyl carrier protein reductase (ENR) catalyzes an
     essential step in fatty acid biosynthesis. ENR is an attractive target
     for narrow-spectrum antibacterial drug discovery because of its essential
     role in metab. and its sequence conservation across many bacterial
     species. In addn., the bacterial ENR sequence and structural organization
     are distinctly different from those of mammalian fatty acid biosynthesis
     enzymes. High-throughput screening to identify inhibitors of Escherichia
     coli ENR yielded four structurally distinct classes of hits. Several
     members of one of these, the 2-(alkylthio)-4,6-diphenylpyridine-3-
     carbonitriles ("thiopyridines"), inhibited both purified ENR (50%
     inhibitory concn. [IC50] = 3-25 .mu.M) and the growth of Staphylococcus
     aureus and Bacillus subtilis (MIC = 1-64 \cdot mu.q/mL). The effect on cell
     growth is due in part to inhibition of fatty acid biosynthesis as judged
     by inhibition of incorporation of [14C]acetate into fatty acids and by the
     increased sensitivity of cells that underexpress an ENR-encoding gene
     (4-8-fold MIC shift). Synthesis of a variety of compds. in this chem.
     series revealed a correlation between IC50 and MIC, and the results
     provided initial structure-activity relationships. Preliminary
     structure-activity relationships, potency on purified ENR, and activity on
     bacterial cells indicate that members of the thiopyridine chem. series are
     effective fatty acid biosynthesis inhibitors suitable for further
```

antibacterial development.

```
ΙT
      ***733052-06-7***
                       , GTC 343130
                                     ***733052-07-8*** , GTC 330346
      ***750595-50-7*** , GTC 343131
    RL: BSU (Biological study, unclassified); BIOL (Biological study)
       (inhibitors of bacterial enoyl-acyl carrier protein reductase)
RN
    296797-06-3 CAPLUS
CN
    Acetamide, N-[3-(acetylamino)phenyl]-2-[(3-cyano-4,6-di-2-thienyl-2-
    pyridinyl)thio] - (CA INDEX NAME)
/ Structure 19 in file .gra /
    340808-61-9 CAPLUS
CN
    Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
    INDEX NAME)
/ Structure 20 in file .gra /
    354555-67-2 CAPLUS
RN
    Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-
CN
    (CA INDEX NAME)
/ Structure 21 in file .gra /
RN
    733052-04-5 CAPLUS
CN
    Benzoic acid, 4-[2-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
    (CA INDEX NAME)
/ Structure 22 in file .gra /
RN
    733052-06-7 CAPLUS
CN
    Benzoic acid, 3-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
    INDEX NAME)
/ Structure 23 in file .gra /
    733052-07-8 CAPLUS
RN
    Benzeneacetic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]-
CN
      (CA INDEX NAME)
/ Structure 24 in file .gra /
RN
    750595-50-7 CAPLUS
CN
    Benzoic acid, 4-[1-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
    (CA INDEX NAME)
/ Structure 25 in file .gra /
REFERENCE COUNT:
                      26
                            THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
                            RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

```
ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        DOCUMENT NUMBER:
                        133:207831
                        Synthesis of substituted 4-hydroxy-1H-thieno[2,3-b;4,5-
TITLE:
                        b']dipyridin-2-ones
AUTHOR(S):
                        Rodinovskaya, L. A.; Shestopalov, A. M.
CORPORATE SOURCE:
                        N. D. Zelinsky Institute of Organic Chemistry, Russian
                        Academy of Sciences, Moscow, 117913, Russia
SOURCE:
                        Russian Chemical Bulletin (Translation of Izvestiya
                        Akademii Nauk, Seriya Khimicheskaya) (2000), 49(2),
                        348-354
                        CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER:
                        Consultants Bureau
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        English
GΙ
/ Structure 26 in file .gra /
     Substituted 4-hydroxy-1H-thieno[2,3-b;4,5-b']dipyridin-2-ones, e.g., I,
AΒ
    were prepd. by reaction of 3-cyanopyridine-2(1H)-thiones with alkyl
     4-chloroacetoacetates and by intramol. cyclization of alkyl
     4-(2-pyridylthio)acetoacetates or alkyl 3-(3-aminothieno[2,3-b]pyridin-2-
    yl)-3-oxopropionates under the action of bases.
      ***243987-05-5***
ΙT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of 4-hydroxy-1H-thieno[2,3-b;4,5-b']dipyridin-2-ones)
     243987-05-5 CAPLUS
     3-Pyridinecarbonitrile, 1,2-dihydro-4,6-di-2-thienyl-2-thioxo- (CA INDEX
CN
    NAME)
/ Structure 27 in file .gra /
      ***290299-69-3P***
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of 4-hydroxy-1H-thieno[2,3-b;4,5-b']dipyridin-2-ones)
     290299-69-3 CAPLUS
RN
    Butanoic acid, 4-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-3-oxo-,
CN
     ethyl ester (CA INDEX NAME)
/ Structure 28 in file .gra /
                              THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                        9
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
                        1999:455705 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        131:228634
TITLE:
                        One stage synthesis of 4,6-diaryl-3-cyanopyridine-
                        2(1H)-thiones
AUTHOR(S):
                        Shestopalov, A. M.; Nikishin, K. G.
```

CORPORATE SOURCE: N. D. Zelinskii Institute of Organic Chemistry,

Russian Academy of Sciences, Moscow, 117913, Russia

SOURCE: Chemistry of Heterocyclic Compounds (New

> York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1093

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal English LANGUAGE:

The title compds. were prepd. in 82-92% yields by cyclization of

.alpha.,.beta.-unsatd. ketones with malononitrile and S in refluxing EtOH

in the presence of morpholine.

ΙT \*\*\*243987-05-5P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of diarylcyanopyridine 2(1H)-thiones)

243987-05-5 CAPLUS RN

3-Pyridinecarbonitrile, 1,2-dihydro-4,6-di-2-thienyl-2-thioxo- (CA INDEX

NAME)

/ Structure 29 in file .gra /

2 REFERENCE COUNT: THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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                 predefined hit display formats
NEWS
     4 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family
                 searching
     7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology
NEWS
                 sequence search option
NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character
                 patent numbers for U.S. applications
NEWS 11 JUN 19 CAS REGISTRY includes selected substances from
                 web-based collections
NEWS 12 JUN 25 CA/Caplus and USPAT databases updated with IPC
                 reclassification data
NEWS 13
        JUN 30 AEROSPACE enhanced with more than 1 million U.S.
                 patent records
        JUN 30
                EMBASE, EMBAL, and LEMBASE updated with additional
NEWS 14
                 options to display authors and affiliated
                 organizations
NEWS 15 JUN 30 STN on the Web enhanced with new STN AnaVist
                 Assistant and BLAST plug-in
NEWS 16 JUN 30 STN AnaVist enhanced with database content from EPFULL
NEWS 17 JUL 28 CA/CAplus patent coverage enhanced
NEWS 18 JUL 28 EPFULL enhanced with additional legal status
                 information from the epoline Register
NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20 JUL 28 STN Viewer performance improved
NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts
                 page images from 1967-1998
NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS 24 AUG 15 CAplus currency for Korean patents enhanced
NEWS 25 AUG 25 CA/Caplus, CASREACT, and IFI and USPAT databases
                 enhanced for more flexible patent number searching
NEWS 26 AUG 27 CAS definition of basic patents expanded to ensure
                 comprehensive access to substance and sequence
                 information
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L1 STRUCTURE UPLOADED
=> d 11
L1 HAS NO ANSWERS
L1
/ Structure 30 in file .gra /
Structure attributes must be viewed using STN Express query preparation.
Uploading C:\Program Files\STNEXP\Queries\10542351 take 4.str
L2 STRUCTURE UPLOADED
=> d 12
L2 HAS NO ANSWERS
/ Structure 31 in file .gra /
Structure attributes must be viewed using STN Express query preparation.
=> s 11 or 12
SAMPLE SEARCH INITIATED 11:32:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 646 TO ITERATE
100.0% PROCESSED 646 ITERATIONS
                                                             11 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                       BATCH **COMPLETE**
PROJECTED ITERATIONS: 11396 TO 14444
PROJECTED ANSWERS:
                              22 TO
                                       418
L3
           11 SEA SSS SAM L1 OR L2
=> s l1 sss full
FULL SEARCH INITIATED 11:32:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 18549 TO ITERATE
100.0% PROCESSED 18549 ITERATIONS
                                                            285 ANSWERS
SEARCH TIME: 00.00.01
L4 285 SEA SSS FUL L1
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=> s 12 sss ful FULL SEARCH INITIATED 11:32:33 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 742 TO ITERATE

100.0% PROCESSED 742 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

L5 2 SEA SSS FUL L2

=> file cap

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ENTRY SESSION 356.72 356.93

FULL ESTIMATED COST

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=> s 14 or 15

100 L4

3 L5

L6 102 L4 OR L5

=> s 16 and bacteria

348391 BACTERIA

129 BACTERIAS

348461 BACTERIA

(BACTERIA OR BACTERIAS)

L7 3 L6 AND BACTERIA

=> d 1-3 17 ibib abs hitstr

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:196524 CAPLUS <<LOGINID::20080908>>

```
DOCUMENT NUMBER:
                                                147:419384
                                                 New antimicrobial 9-(p-heterocyclo-substituted
TITLE:
                                                 anilino) -tetrahydroacridines
                                                 Ebeid, M. Y.; Kamel, M. M.; Nofal, Z. M.; Ragab, F.;
AUTHOR(S):
                                                 Zaghary, W. A.; El-Kady, M.
CORPORATE SOURCE:
                                                 Faculty of Pharmacy, Cairo University, Egypt
SOURCE:
                                                 Egyptian Journal of Chemistry (2006), 49(2), 277-285
                                                 CODEN: EGJCA3; ISSN: 0449-2285
PUBLISHER:
                                                 National Information and Documentation Centre
DOCUMENT TYPE:
                                                 Journal
LANGUAGE:
                                                 English
         A new series of 9-[p-(4-aryl-3-cyano-2-iminopyridin-6-yl)anilino]-
         1,2,3,4-tetrahydroacridines and their 2-oxo-(or thioxo)-pyridinylanilino
         derivs. were synthesized and evaluated against
                                                                                                          ***bacteria***
          fungi. These compds. showed high significant activity against
          Saccharomyces cerevisiae, Bacillus subtilis, Staphylococcus aureus,
          Penicillium notatum, Aspergillus niger, Candida utilis, and Candida
         albicans.
            ***951320-46-0P***
ΤТ
         RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
         preparation); BIOL (Biological study); PREP (Preparation)
                (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
               tetrahydroacridines)
          951320-46-0 CAPLUS
RN
CN
          3-Pyridinecarbonitrile, 1,2-dihydro-4-phenyl-6-[4-[(1,2,3,4-tetrahydro-9-
          acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 32 in file .gra /
             ***951320-47-1P***
                                                        ***951320-48-2P***
                                                                                                        ***951320-49-3P***
         RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
               tetrahydroacridines)
RN
         951320-47-1 CAPLUS
         3-Pyridinecarbonitrile, 1, 2-dihydro-4-(3-methoxyphenyl)-6-[4-[(1, 2, 3, 4-
CN
          tetrahydro-9-acridinyl)amino|phenyl|-2-thioxo- (CA INDEX NAME)
/ Structure 33 in file .gra /
          951320-48-2 CAPLUS
RN
         3-Pyridinecarbonitrile, 4-(3-\text{chlorophenyl})-1, 2-\text{dihydro}-6-[4-[(1,2,3,4-
CM
          tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 34 in file .gra /
RN
         951320-49-3 CAPLUS
          3-Pyridine carbonitrile, 1,2-dihydro-6-[4-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-14-[(1,2,3,4-tetrahydro-9-1
          acridinyl)amino]phenyl]-2-thioxo-4-(2,3,4-trimethoxyphenyl)- (CA INDEX
         NAME)
/ Structure 35 in file .gra /
ΤТ
            ***951320-50-6***
```

```
RL: RCT (Reactant); RACT (Reactant or reagent)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahydroacridines)
     951320-50-6 CAPLUS
RN
     3-Pyridinecarbonitrile, 4-[3-(dimethylamino)phenyl]-1,2-dihydro-6-[4-
CN
     [(1,2,3,4-tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 36 in file .gra /
REFERENCE COUNT:
                         20
                               THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
     ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1999:221628 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         130:325083
TITLE:
                         Synthesis and antimicrobial activity of some new
                         4-methylquinolines
                         Kamel, M. M.; Fathala, O. A.; Abdou, W. A. M.; Haiba,
AUTHOR(S):
CORPORATE SOURCE:
                         Medicinal Chemistry Department, National Research
                         Centre, Cairo, Egypt
                         Proceedings of the Pakistan Academy of Sciences
SOURCE:
                         (1997), 34(1), 7-11
                         CODEN: PKSPAW; ISSN: 0377-2969
                         Pakistan Academy of Sciences
PUBLISHER:
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridine-6-
     yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinoline
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
               ***bacteria*** , yeast, and fungi. Two compds. showed activity
     against
     against these microorganisms.
                             ***218272-68-5P***
                                                    ***218272-69-6P***
       ***218272-67-4P***
ΤT
       ***223697-02-7P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of methylquinolines as antibacterial and antifungal agents)
RN
     218272-67-4 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 37 in file .gra /
     218272-68-5 CAPLUS
RN
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 38 in file .gra /
RN
     218272-69-6 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
```

```
/ Structure 39 in file .gra /
     223697-02-7 CAPLUS
RN
     3-Pyridinecarbonitrile, 6-[4-[(7-chloro-4-methyl-2-
CN
     quinolinyl)amino]phenyl]-1,2-dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA
     INDEX NAME)
/ Structure 40 in file .gra /
REFERENCE COUNT:
                         17
                               THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
T.7
     ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1998:702455 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         130:66375
TITLE:
                         Synthesis of some new 4-methylquinolines of possible
                         biological activity
                         Kamel, M. M.; Fathalla, O. A.; Abdou, W. A. M.; Omer,
AUTHOR(S):
                         M. T.; Haiba, M. E.
                         Medicinal Chemistry Department, National Research
CORPORATE SOURCE:
                         Centre, Cairo, Egypt
SOURCE:
                         Egyptian Journal of Pharmaceutical Sciences (1998),
                         Volume Date 1997, 38(1-3), 79-86
                         CODEN: EJPSBZ; ISSN: 0301-5068
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridin-6-
     yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinolines
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
              ***bacteria*** , yeast, and fungi. 7-Chloro-4-methyl-2-[4-
     hydroxy-3,5-di(diethylaminomethyl)]anilinoquinoline showed fungicidal
     activity against Aspergillus niger.
       ***218272-67-4P***
                             ***218272-68-5P***
                                                     ***218272-69-6P***
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis and antimicrobial activity of 4-methylquinolines)
     218272-67-4 CAPLUS
RN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
CN
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 41 in file .gra /
RN
     218272-68-5 CAPLUS
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
CN
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 42 in file .gra /
     218272-69-6 CAPLUS
RN
CN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
```

/ Structure 43 in file .gra /

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file stnq

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 21.83 378.76 SINCE FILE TOTAL ENTRY SESSION DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) -2.40 -2.40 CA SUBSCRIBER PRICE

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SINCE FILE TOTAL ENTRY SESSION 0.00 CA SUBSCRIBER PRICE -2.40

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STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 New CAS Information Use Policies, enter HELP USAGETERMS for details.

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS

L8 STF

/ Structure 44 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 18 sss ful

FULL SEARCH INITIATED 11:49:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1468 TO ITERATE

100.0% PROCESSED 1468 ITERATIONS

16 ANSWERS

SEARCH TIME: 00.00.01

L9 16 SEA SSS FUL L8

=> file cap

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
178.36 558.32

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY
SESSION
CA SUBSCRIBER PRICE

0.00 -2.40

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FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

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=> s 19 L10 5 L9

=> d 110 1-5 ibib abs hitstf 'HITSTF' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ---- GI and AB ALL ----- BIB, AB, IND, RE APPS ----- AI, PRAI BIB ----- AN, plus Bibliographic Data and PI table (default) CAN ----- List of CA abstract numbers without answer numbers CBIB ----- AN, plus Compressed Bibliographic Data CLASS ----- IPC, NCL, ECLA, FTERM DALL ----- ALL, delimited (end of each field identified) DMAX ----- MAX, delimited for post-processing FAM ----- AN, PI and PRAI in table, plus Patent Family data FBIB ----- AN, BIB, plus Patent FAM IND ----- Indexing data IPC ----- International Patent Classifications MAX ----- ALL, plus Patent FAM, RE PATS ----- PI, SO SAM ----- CC, SX, TI, ST, IT SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;

SCAN must be entered on the same line as the DISPLAY, e.g., D SCAN or DISPLAY SCAN)

STD ----- BIB, CLASS

IABS ----- ABS, indented with text labels IALL ----- ALL, indented with text labels IBIB ----- BIB, indented with text labels IMAX ----- MAX, indented with text labels ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original) OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations

SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms

HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)

containing hit terms

HITRN ----- HIT RN and its text modification

HITSTR ----- HIT RN, its text modification, its CA index name, and

its structure diagram

HITSEQ ----- HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields

FHITSTR ---- First HIT RN, its text modification, its CA index name, and

its structure diagram

FHITSEQ ---- First HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields

KWIC ----- Hit term plus 20 words on either side

OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI, AU; BIB, ST; TI, IND; TI, SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number. ENTER DISPLAY FORMAT (BIB):end

## => d 110 1-5 ibib abs hitstr

L10 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:798258 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 148:538031

TITLE: Synthesis and investigation of the stability of esters

of 6'-carbamoylmethylthio-5'-cyano-1',4'-dihydro-3,4'-

and -4,4'-bipyridine-3'-carboxylic acids. Part 1. Esters of 6'-carbamoylmethylthio-5'-cyano-1',4'-

dihydro-3,4'-bipyridine-3'-carboxylic acids

AUTHOR(S): Kazoka, H.; Krauze, A.; Vilums, M.; Cernova, L.; Sile,

L.; Duburs, G.

CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV-1006,

Latvia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY,

United States) (2007), 43(1), 50-57

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Esters of 6'-carbamoylmethylthio-5'-cyano-1',4'-dihydro-3,4'-bipyridine-3'-carboxylic acids are obtained by the alkylation of piperidinium 3'-alkoxycarbonyl-5'-cyano-1',4'-dihydro-3,4'-bipyridine-6'-thiolates with iodoacetamide. For an HPLC study of the stability of solns. of the abovementioned 1,4-dihydrobipyridines (soln., pH 2.3-9.0), the appropriate esters of 6'-carbamoylmethylthio-5'-cyano-3,4'-bipyridine-3'-carboxylic acids and esters of 8-cyano-5-methyl(or phenyl)-3-oxo-7-pyridin-3-yl-2,3-dihydro-7H-thiazolo[3,2-a]pyridine-6-carboxylic acids were synthesized as

ref. compds. Anal. by HPLC was carried out under conditions of reverse-phase chromatog. It was shown that solns. of the investigated compds. in a mixt. of MeCN and phosphate buffer (pH 3.0-5.0) were stable for 1 mo on storage protected from light. Under the action of light in all the solns. investigated irresp. of pH, the formation occurs of the corresponding esters of 6'-carbamoylmethylthio-5'-cyano-3,4'-bipyridine-3'carboxylic acids. The presence of esters of 8-cyano-5-methyl(or phenyl)-3-oxo-7-pyridin-3-yl-2,3-dihydro-7H-thiazolo[3,2-a]pyridine-6carboxylic acids (.ltoreq.4%) was detected only in 0.1% solns. of phosphoric acid (pH 2.3) under conditions of storage of the latter protected from light. A series of as yet unidentified products was detected in solns. of pH 7.0-9.0. \*\*\*144969-93-7P\*\*\* RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and stability of esters of (carbamoylmethylthio)cyanodihydrobip yridinecarboxylates) 144969-93-7 CAPLUS [3,4'-Bipyridine]-3'-carboxylic acid, 6'-[(2-amino-2-oxoethyl)thio]-5'cyano-2'-phenyl-, ethyl ester (CA INDEX NAME) / Structure 45 in file .gra / REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT L10 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1999:547305 CAPLUS <<LOGINID::20080908>> DOCUMENT NUMBER: 131:295109 Derivatives of 3-cyano-6-phenyl-4-(3'-pyridyl)-TITLE: pyridine-2(1H)-thione and their neurotropic activity Krauze, Aivars; Germane, Skaidrite; Eberlins, Ojars; AUTHOR(S): Sturms, Igors; Klusa, Vija; Duburs, Gunars CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV-1006, Latvia European Journal of Medicinal Chemistry (1999), 34(4), SOURCE: 301-310 CODEN: EJMCA5; ISSN: 0223-5234 PUBLISHER: Editions Scientifiques et Medicales Elsevier DOCUMENT TYPE: Journal LANGUAGE: English 3-Cyano-6-phenyl-4-(3'-pyridyl)pyridine-2(1H)-thione, the related2,2'-bis-pyridyldisulfide, 2-alkylthiopyridines and 2-amino-thieno[2,3b]pyridines were synthesized and their neurotropic activities were examd. Bispyridyldisulfide exhibited low toxicity (LD50 > 5000 mg/kg, ICR mice, i.p.) and selective antiamnesic activity at the doses of 0.05-0.5~mg/kgp.o. This effect was significantly higher than that induced by Piracetam at 50 mg/kg. \*\*\*247056-20-8P\*\*\* \*\*\*247056-23-1P\*\*\* \*\*\*247056-24-2P\*\*\* \*\*\*247056-25-3P\*\*\* \*\*\*247056-26-4P\*\*\* \*\*\*247056-27-5P\*\*\* \*\*\*247056-28-6P\*\*\* RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-

ΙT

RN

CN

ΙT

pyridine-2(1H)-thione derivs.)

```
247056-20-8 CAPLUS
RN
     [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-phenyl-2'-thioxo- (CA
CN
     INDEX NAME)
/ Structure 46 in file .gra /
RN
     247056-23-1 CAPLUS
CN
     [3,4'-Bipyridine]-3'-carbonitrile, 2'-(methylthio)-6'-phenyl- (CA INDEX
     NAME)
/ Structure 47 in file .gra /
RN
     247056-24-2 CAPLUS
    [3,4'-Bipyridine]-3'-carbonitrile, 2'-(ethylthio)-6'-phenyl- (CA INDEX
CN
    NAME)
/ Structure 48 in file .gra /
     247056-25-3 CAPLUS
RN
    Acetic acid, 2-[(3'-cyano-6'-phenyl[3,4'-bipyridin]-2'-yl)thio]-, ethyl
CN
     ester (CA INDEX NAME)
/ Structure 49 in file .gra /
RN
     247056-26-4 CAPLUS
     [3,4'-Bipyridine]-3'-carbonitrile, 2'-[(cyanomethyl)thio]-6'-phenyl- (CA
CN
     INDEX NAME)
/ Structure 50 in file .gra /
     247056-27-5 CAPLUS
RN
CN
     Acetamide, 2-[(3'-cyano-6'-phenyl[3,4'-bipyridin]-2'-yl)thio]- (CA INDEX
/ Structure 51 in file .gra /
     247056-28-6 CAPLUS
RN
     [3,4'-Bipyridine]-3'-carbonitrile, 2'-[(2-oxo-2-phenylethyl)thio]-6'-
CN
     phenyl- (CA INDEX NAME)
/ Structure 52 in file .gra /
      ***247056-21-9P***
ΙT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-
       pyridine-2(1H)-thione derivs.)
     247056-21-9 CAPLUS
RN
```

```
[3,4'-Bipyridine]-3'-carbonitrile, 2',2'''-dithiobis[6'-phenyl- (9CI) (CA
CM
     INDEX NAME)
/ Structure 53 in file .gra /
       ***247056-22-0P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-
        pyridine-2(1H)-thione derivs.)
RN
     247056-22-0 CAPLUS
CN
    [3,4'-Bipyridine]-3'-carbonitrile, 6'-phenyl-2'-(1-piperidinylthio)- (CA
     INDEX NAME)
/ Structure 54 in file .gra /
REFERENCE COUNT:
                         48
                               THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L10 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
                         1993:38791 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
                         118:38791
DOCUMENT NUMBER:
ORIGINAL REFERENCE NO.: 118:7067a,7070a
                         Synthesis, properties, and cardiotonic activity of
TITLE:
                         2-carbamoylmethylthio-6-phenyl-5-ethoxycarbonyl-3-
                         cyclo-4-(pyrido-3'yl)pyridine derivatives and their
                         hydrogenated analogs
AUTHOR(S):
                         Krauze, A.; Garalene, V.; Duburs, G.
                         Inst. Org. Synth., Riga, Latvia
CORPORATE SOURCE:
SOURCE:
                         Khimiko-Farmatsevticheskii Zhurnal (1992), 26(5), 40-3
                        CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        Russian
GΙ
/ Structure 55 in file .gra /
AB
     Cyclocondensation of PhCOCH2CO2Et with 2-cyano-3-pyridinethioacrylamide in
     the presence of bases gave pyridinecarboxylates I (X+ = piperidino, Na)
     which when treated with ICH2CONH2 gave 82% amide II; betaine III (R = H)
     similarly treated gave amide III (R = CH2CONH2) which underwent
     base-catalyzed cyclization to give thienopyridine IV (R1 = 3-pyridyl).
     Addnl. obtained was IV (R1 = Ph). The 4,3'-bipyridines show dual
     activity-neg. inotropic action at low concns. and pos. inotropic activity
     at concns. >10-5M.
      ***144969-93-7P***
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., cyclization, and cardiotonic properties of)
RN
     144969-93-7 CAPLUS
CN
     [3,4'-Bipyridine]-3'-carboxylic acid, 6'-[(2-amino-2-oxoethyl)thio]-5'-
     cyano-2'-phenyl-, ethyl ester (CA INDEX NAME)
```

```
/ Structure 56 in file .gra /
L10 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1990:515227 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         113:115227
ORIGINAL REFERENCE NO.: 113:19527a,19530a
TITLE:
                         Polycyclic pyridines. Part 8. Synthesis of new
                         primary, secondary and tertiary 3-aminothieno[2,3-
                         b]pyridine-2-carboxamides by different pathways
AUTHOR (S):
                         Wagner, G.; Vieweg, H.; Leistner, S.; Boehm, N.;
                         Krasselt, U.; Hanfeld, Vera; Prantz, J.; Grupe, Renate
CORPORATE SOURCE:
                         Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010,
                         Ger. Dem. Rep.
SOURCE:
                         Pharmazie (1990), 45(2), 102-9
                         CODEN: PHARAT; ISSN: 0031-7144
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                        German
OTHER SOURCE(S):
                        CASREACT 113:115227
GΙ
/ Structure 57 in file .gra /
     The treatment of 2-thioxo-1,2-dihydropyridine-3-carbonitriles with
AB
     C1CH2CO2NR1R3 (R1, R2 = H, Me, Et) gave 3-aminothieno[2,3-
     b]pyridinecarboxylic acid amides I [R1 = H, Et, Me; R2 = H, Et, Bu,
     cyclohexyl, CH2CH2OH, CH2CO2H; R1R2 = (CH2)5; R3 = Me, Ph, 4-BrC6H4,
     3-\text{pyridyl}, CONH2, etc; R4 = H, Me, CH2C6H4(CN)-4; R5 = Me, C6H4Cl-4, Ph,
     C6H4Br-4, furyl, naphthyl, OH). Some of the compds. thus prepd., e.g. I
     (R1 = R2 = R4 = H, R3 = Me, R5 = Ph) and I (R1 = R4 = H, R2 = CH2CH2OH, R3)
     = R5 = Me) showed activity as antiallergics in the passive cutaneous
     anaphylaxis test in rats.
       ***127144-07-4***
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (condensation reaction of, with chloroacetamide)
     127144-07-4 CAPLUS
RN
     [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-(2-naphthalenyl)-2'-
CN
     thioxo- (CA INDEX NAME)
/ Structure 58 in file .gra /
L10 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1990:216643 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         112:216643
ORIGINAL REFERENCE NO.: 112:36565a,36568a
TITLE:
                         Multicyclic pyridines. Part 6. Synthesis of new
                         heterocycle substituted 2-thioxo-1,2-dihydropyridine-3-
                         carbonitriles
AUTHOR(S):
                         Vieweg, H.; Hanfeld, Vera; Leistner, S.; Wagner, G.
CORPORATE SOURCE:
                         Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010,
                         Ger. Dem. Rep.
```

Pharmazie (1989), 44(9), 639-40 CODEN: PHARAT; ISSN: 0031-7144

SOURCE:

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 112:216643

GΙ

/ Structure 59 in file .gra /

AB Condensation of R1COMe (R1 = 2-furyl, 2-thienyl, 2-naphthyl) with R2CHO (R2 = Ph, 4-FC6H4, 4-ClC6H4, 4-BrC6H4, 3-pyridyl) in MeOH or H2O contg. NaOH gave 45-88% R1COCH:CHR2 which on cyclocondensation with NH2CSCH2CN in the presence of NaOMe in MeOH gave 32-71% title compds. I. Cyclocondensation of 1-(2-thienyl)-1,3-butanedione with NH2CSCH2CN in the presence of K2CO3-Me2CO gave isomeric mixt. of I (R1 = 2-thienyl, R2 = Me; R1 = Me, R2 = 2-thienyl) which on condensation with ClCH2CO2Et followed by base-mediated cyclization gave thienopyridinecarboxylates II (R3 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl).

TT \*\*\*127144-07-4P\*\*\*

RN 127144-07-4 CAPLUS

CN [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-(2-naphthalenyl)-2'-thioxo- (CA INDEX NAME)

/ Structure 60 in file .gra /

=> file reg

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http://www.cas.org/support/stngen/stndoc/properties.html

=>

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L11 STRUCTURE UPLOADED

=> d 111

L11 HAS NO ANSWERS

L11 STR

/ Structure 61 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=>

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L12 STRUCTURE UPLOADED

=> d 112

L12 HAS NO ANSWERS

L12 STR

/ Structure 62 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 111 sss sam

SAMPLE SEARCH INITIATED 11:54:10 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2127 TO ITERATE

94.0% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 39774 TO 45306 PROJECTED ANSWERS: 38498 TO 43944

L13 50 SEA SSS SAM L11

=> s 111 sss ful

FULL SEARCH INITIATED 11:54:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 41604 TO ITERATE

100.0% PROCESSED 41604 ITERATIONS

SEARCH TIME: 00.00.01

40140 ANSWERS

50 ANSWERS

=> s 112 sss ful

FULL SEARCH INITIATED 11:55:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 51043 TO ITERATE

100.0% PROCESSED 51043 ITERATIONS

2250 ANSWERS

SEARCH TIME: 00.00.01

L15 2250 SEA SSS FUL L12

=> file cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

357.64 FULL ESTIMATED COST 946.09

SINCE FILE TOTAL ENTRY SESSION DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 114 or 115

1101 L14

765 L15

1125 L14 OR L15 L16

=> d l16 and bacteria

<sup>&#</sup>x27;AND' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

<sup>&#</sup>x27;BACTERIA' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

```
ABS ---- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, CLASS
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ---- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
             containing hit terms
\mbox{\sc HITRN} ----- \mbox{\sc HIT} \mbox{\sc RN} and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
            its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
             its structure diagram
FHITSEQ ---- First HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
```

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number. ENTER DISPLAY FORMAT (BIB):end => s 116 and bacteria 348391 BACTERIA 129 BACTERIAS 348461 BACTERIA (BACTERIA OR BACTERIAS) L17 11 L16 AND BACTERIA => d scan T.17 11 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN IC ICM C07D519-00 ICA A61K031-545 ICI C07D519-00, C07D501-00, C07D495-00 26-5 (Biomolecules and Their Synthetic Analogs) Section cross-reference(s): 1 Preparation of cephalosporin derivatives as antibacterial agents TIST thienopyridiniomethylcephemcarboxylate prepn antibacterial; cephalosporin prepn antibacterial; cephemcarboxylate thienopyridiniomethyl prepn antibacterial ΤТ Antibiotics ([thiazolyl(hydroxyimino)acetamido](thienopyridiniomethyl)cephemcarboxy late derivs.) 152938-72-2P 152938-73-3P 152938-75-5P ΙT 152938-71-1P 152938-74-4P 152938-76-6P 152938-77-7P 152938-78-8P 152938-79-9P 152938-80-2P 152938-82-4P 152938-81-3P 152938-83-5P 152938-84-6P 152938-85-7P 152938-86-8P 152938-87-9P 152938-88-0P 152938-89-1P 152938-90-4P 152938-91-5P 152938-92-6P 152938-93-7P 152938-94-8P 152938-95-9P 152938-96-0P 152938-97-1P 152938-98-2P 152938-99-3P 152939-00-9P 152939-01-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. of, as antibacterial agent) 152938-45-9P 151027-96-2P 151027-97-3P 152938-44-8P ΤТ 152938-46-0P 152938-47-1P 152938-48-2P 152938-49-3P 152938-50-6P 152938-51-7P 152938-52-8P 152938-53-9P 152938-54-0P 152938-55-1P 152938-56-2P 152938-57-3P 152938-58-4P 152938-59-5P 152938-60-8P 152938-61-9P 152938-62-0P 152938-63-1P 152938-65-3P 152938-64-2P 152938-66-4P 152938-67-5P 152938-68-6P 152938-69-7P 152938-70-0P 152939-02-1P 152939-03-2P 152939-04-3P 152939-05-4P 152939-06-5P 152939-07-6P 152939-10-1P 152939-08-7P 152939-09-8P \*\*\*152939-11-2P\*\*\* \*\*\*152939-12-3P\*\*\* 152939-13-4P 152939-14-5P, Thieno[2,3b]pyridine-3,5-diamine 152939-15-6P 152939-16-7P 152939-17-8P 152939-18-9P 152939-19-0P 152939-22-5P 152939-20-3P 152939-21-4P 152939-23-6P 152939-24-7P 152939-25-8P 152939-26-9P 152939-27-0P 152939-28-1P 152939-29-2P 152939-30-5P 152939-32-7P RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as intermediate for antibacterial cephalosporin deriv.) 75-52-5, Nitromethane, reactions 105-36-2, Ethyl bromoacetate

407-25-0, Trifluoroacetic anhydride 563-41-7, Semicarbazide hydrochloride 762-49-2, 1-Bromo-2-fluoroethane 883-40-9,

Diphenyldiazomethane 2365-48-2, Methyl thioglycolate 7664-41-7, Ammonia, reactions 18600-39-0, Cyclopropylamine hydrochloride 24424-99-5, Di-tert-butyl dicarbonate 26579-54-4, Thieno[2,3-b]pyridin-3-31309-08-7 53174-99-5, 3-Formylthieno[2,3-b]pyridine amine 142604-12-4 152939-31-6, Thieno[2,3-b]pyridin-3-ol 84728-65-4 152939-33-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in prepn. of antibacterial cephalosporin deriv.)

11111-12-9D, Cephalosporin, derivs. ΤТ

> RL: RCT (Reactant); RACT (Reactant or reagent) (thienopyridiniomethyl-)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

## => d 117 1-11 ibib abs hitstr

L17 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2008:526897 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 149:121710

TITLE: Virtual screening and experimental verification to

identify potential inhibitors of the ErmC

methyltransferase responsible for bacterial resistance

against macrolide antibiotics

AUTHOR(S): Feder, Marcin; Purta, Elzbieta; Koscinski, Lukasz;

Cubrilo, Sonja; Vlahovicek, Gordana Maravic; Bujnicki,

Janusz M.

CORPORATE SOURCE: Laboratory of Bioinformatics and Protein Engineering,

International Institute of Molecular and Cell Biology,

Warsaw, 02109, Pol.

SOURCE: ChemMedChem (2008), 3(2), 316-322

CODEN: CHEMGX; ISSN: 1860-7179

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

Methyltransferases from the Erm family catalyze S-adenosyl-L-methioninedependent modification of a specific adenine residue in bacterial 23S rRNA, thereby conferring resistance to clin. important macrolide, lincosamide, and streptogramin B antibiotics. Thus, far, no inhibitors of these enzymes have been identified or designed that would effectively abolish the resistance in vivo. We used the crystal structure of ErmC' methyltransferase as a target for structure-based virtual screening of a database composed of 58679 lead-like compds. Among 77 compds. selected for exptl. validation (63 predicted to bind to the catalytic pocket and 14 compds. predicted to bind to the putative RNA binding site), we found several novel inhibitors that decrease the minimal inhibitory concn. of a macrolide antibiotic erythromycin toward an Escherichia coli strain that constitutively expresses ErmC'. Eight of them have IC50 values in the micromolar range. Anal. of docking models of the identified inhibitors suggests a novel strategy to develop potent and clin. useful inhibitors. ΤТ

\*\*\*285987-27-1\*\*\*

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(ErmC' methyltransferase inhibitor; virtual screening and exptl. verification to identify potential inhibitors of ErmC methyltransferase responsible for bacterial resistance against macrolide antibiotics)

RN 285987-27-1 CAPLUS

3-Pyridinecarbonitrile, 4-methyl-2,6-bis[(4-methylphenyl)thio]- (CA INDEX CN

NAME)

```
/ Structure 63 in file .gra /
REFERENCE COUNT:
                         26
                               THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2007:436667 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         147:469291
TITLE:
                         A convenient synthesis of some new
                         indeno[1,2-b]pyridines and indeno[1,2-b]thieno[3,2-
                         e]pyridine derivatives with potential biological
                         activity
                         El-Ossaily, Yasser A.
AUTHOR(S):
CORPORATE SOURCE:
                         Chemistry Department, Assiut University, Assiut, Egypt
SOURCE:
                         Phosphorus, Sulfur and Silicon and the Related
                         Elements (2007), 182(5), 1109-1117
                         CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER:
                         Taylor & Francis, Inc.
DOCUMENT TYPE:
                         Journal
                         English
LANGUAGE:
OTHER SOURCE(S):
                        CASREACT 147:469291
GT
/ Structure 64 in file .gra /
     Heterocyclization of 1,3-indandione with arylidene cyanoacetamide, or
AB
     arylideneindanone with cyanoacetamide afforded indenopyridinethione, which
     underwent cyclization with Et chloroacetate or chloroacetone to give
     indenothienopyridines. The alkylthioindenopyridines. underwent ring
     closure with sodium ethoxide to produce aminoindenothienopyridines, e.g.,
     I. The indenothienopyridinecarbonitriles underwent heterocyclization with
     carbon disulfide in pyridine to give indenopyridinothienopyrimidines,
     e.g., II. Most of the synthesized compds. were screened in vitro for
     their antimicrobial activities against four species of
                                                              ***bacteria***
     and six species of fungi using chloramphenicol and terbinafine as stds.
       ***311767-75-6P***
                              ***952720-95-5P***
                                                     ***952720-97-7P***
ΤТ
                              ***952720-99-9P***
       ***952720-98-8P***
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant
     or reagent)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene) indandiones using heterocyclization as
        key step)
     311767-75-6 CAPLUS
RN
CN
     1H-Indeno[1,2-b]pyridine-3-carbonitrile, 2,5-dihydro-5-oxo-4-(2-thienyl)-2-
     thioxo- (CA INDEX NAME)
/ Structure 65 in file .gra /
```

```
952720-95-5 CAPLUS
RN
CN
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 2-[(cyanomethyl)thio]-5-oxo-4-(2-
     thienyl) - (CA INDEX NAME)
/ Structure 66 in file .gra /
     952720-97-7 CAPLUS
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 5-oxo-2-[(2-oxo-2-
CN
     phenylethyl)thio]-4-(2-thienyl)- (CA INDEX NAME)
/ Structure 67 in file .gra /
     952720-98-8 CAPLUS
    Acetamide, 2-[[3-cyano-5-oxo-4-(2-thienyl)-5H-indeno[1,2-b]pyridin-2-
     yl]thio]- (CA INDEX NAME)
/ Structure 68 in file .gra /
     952720-99-9 CAPLUS
RN
     Acetamide, 2-[[3-cyano-5-oxo-4-(2-thienyl)-5H-indeno[1,2-b]]pyridin-2-
     yl]thio]-N-(4-methoxyphenyl)- (CA INDEX NAME)
/ Structure 69 in file .gra /
ΙT
       ***952720-93-3P***
                            ***952720-94-4P***
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene)indandiones using heterocyclization as
        key step)
     952720-93-3 CAPLUS
RN
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 2-(methylthio)-5-oxo-4-(2-
CN
     thienyl) - (CA INDEX NAME)
/ Structure 70 in file .gra /
RN
     952720-94-4 CAPLUS
CN
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 2-(ethylthio)-5-oxo-4-(2-thienyl)-
       (CA INDEX NAME)
/ Structure 71 in file .gra /
       ***952720-96-6P***
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene)indandiones using heterocyclization as
        key step)
```

```
RN
     952720-96-6 CAPLUS
CN
     Acetamide, N-(4-chlorophenyl)-2-[[3-cyano-5-oxo-4-(2-thienyl)-5H-
     indeno[1,2-b]pyridin-2-yl]thio]- (CA INDEX NAME)
/ Structure 72 in file .gra /
ΤТ
       ***952721-00-5P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene)indandiones using heterocyclization as
        key step)
RN
     952721-00-5 CAPLUS
CM
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 5-oxo-2-[(phenylmethyl)thio]-4-(2-
     thienyl) - (CA INDEX NAME)
/ Structure 73 in file .gra /
REFERENCE COUNT:
                               THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
                         13
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        2007:196524 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         147:419384
TITLE:
                         New antimicrobial 9-(p-heterocyclo-substituted
                         anilino)-tetrahydroacridines
                         Ebeid, M. Y.; Kamel, M. M.; Nofal, Z. M.; Ragab, F.;
AUTHOR(S):
                         Zaghary, W. A.; El-Kady, M.
CORPORATE SOURCE:
                         Faculty of Pharmacy, Cairo University, Egypt
SOURCE:
                         Egyptian Journal of Chemistry (2006), 49(2), 277-285
                         CODEN: EGJCA3; ISSN: 0449-2285
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     A new series of 9-[p-(4-aryl-3-cyano-2-iminopyridin-6-yl)anilino]-
     1,2,3,4-tetrahydroacridines and their 2-oxo-(or thioxo)-pyridinylanilino
     derivs. were synthesized and evaluated against
                                                     ***bacteria***
     fungi. These compds. showed high significant activity against
     Saccharomyces cerevisiae, Bacillus subtilis, Staphylococcus aureus,
     Penicillium notatum, Aspergillus niger, Candida utilis, and Candida
     albicans.
       ***951320-46-0P***
ΙT
     RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahydroacridines)
RN
     951320-46-0 CAPLUS
     3-Pyridine carbonitrile, 1,2-dihydro-4-phenyl-6-[4-[(1,2,3,4-tetrahydro-9-index)]
CN
     acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 74 in file .gra /
ΙT
       ***951320-47-1P***
                             ***951320-48-2P***
                                                     ***951320-49-3P***
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
```

```
(new antimicrobial 9-(p-heterocyclo-substituted anilino)-
       tetrahydroacridines)
     951320-47-1 CAPLUS
RN
     3-Pyridinecarbonitrile, 1,2-dihydro-4-(3-methoxyphenyl)-6-[4-[(1,2,3,4-
CN
     tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 75 in file .gra /
RN
    951320-48-2 CAPLUS
     3-Pyridinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-[4-[(1,2,3,4-
    tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 76 in file .gra /
RN
    951320-49-3 CAPLUS
    3-Pyridinecarbonitrile, 1,2-dihydro-6-[4-[(1,2,3,4-tetrahydro-9-
     acridinyl)amino]phenyl]-2-thioxo-4-(2,3,4-trimethoxyphenyl)- (CA INDEX
    NAME)
/ Structure 77 in file .gra /
      ***951320-50-6***
ΤТ
    RL: RCT (Reactant); RACT (Reactant or reagent)
       (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
       tetrahydroacridines)
     951320-50-6 CAPLUS
RN
     3-Pyridinecarbonitrile, 4-[3-(dimethylamino)phenyl]-1,2-dihydro-6-[4-
CN
     [(1,2,3,4-tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 78 in file .gra /
                              THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                        20
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
                       2003:971725 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        Transcription factor modulating compounds and methods
TITLE:
                        of use thereof
INVENTOR(S):
                        Levy, Stuart B.; Alekshun, Michael N.; Podlogar, Brent
                        L.; Ohemeng, Kwasi; Verma, Atul K.; Warchol, Tadeusz;
                        Bhatia, Beena
PATENT ASSIGNEE(S):
                        USA
                        U.S. Pat. Appl. Publ., 301 pp.
SOURCE:
                        CODEN: USXXCO
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:
    PATENT NO.
                       KIND DATE
                                          APPLICATION NO. DATE
                        ____
    US 20030229065 A1
                               20031211
                                          US 2002-139591
                                                                  20020814
```

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20021104
                                        CA 2002-2445515
    CA 2445515
                        A1
                                                                 20020506
                                         WO 2002-US14255
    WO 2004001058
                         Α2
                               20031231
                                                                 20020506
    WO 2004001058
                        A3
                               20050303
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
            GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
            GN, GQ, GW, ML, MR, NE, SN, TD, TG
    AU 2002367953
                        Α1
                               20040106
                                        AU 2002-367953
    AU 2002367953
                         В2
                               20080717
    EP 1524974
                         A2
                               20050427
                                         EP 2002-807554
                                                                 20020506
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                        Τ
                               20050707 JP 2004-515557
    JP 2005519998
                                                                 20020506
     US 20050124678
                        A1
                               20050609
                                          US 2003-700661
                                                                 20031103
                               20080729
    US 7405235
                        В2
                                          AU 2008-203017
    AU 2008203017
                        A1
                               20080731
                                                                 20080708
                                                            P 20010504
A3 20020506
                                          US 2001-288660P
PRIORITY APPLN. INFO.:
                                           AU 2002-367953
                                           WO 2002-US14255
                                                             W 20020506
                                                             A2 20020814
                                           US 2002-139591
                                           US 2002-423319P
                                                            P 20021101
                                          US 2002-425916P P 20021113
OTHER SOURCE(S):
                        MARPAT 140:35893
    Methods for identifying compd. useful as anti-infectives that decrease
     resistance, virulence, or growth of microbes are provided. In one
     embodiment, the method comprises contacting a microbial cell comprising:
     (1) a selectable marker under the control of a transcription factor
    responsive element and (2) a transcription factor, with a compd. under
     conditions which allow interaction of the compd. with the microbial cell;
     and measuring the ability of the compd. to affect the growth or survival
     of the microbial cell as an indication of whether the test compd.
    modulates the activity of a transcription factor.
     ΤТ
    RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (transcription factor modulating compds. as anti-infectives agents that
       decrease resistance and virulence and growth identified by detg. marker
       under control of responsive element)
RN
     221179-01-7 CAPLUS
CN
     3,5-Pyridinedicarbonitrile, 2-amino-4-(4-hydroxyphenyl)-6-[2-oxo-2-(2-oxo-
     2H-1-benzopyran-3-yl)ethyl]thio]- (CA INDEX NAME)
/ Structure 79 in file .gra /
RN
     299198-34-8 CAPLUS
CN
     3-Pyridinecarbonitrile, 2-[(2-cyclopropyl-2-oxoethyl)thio]-6-(2-thienyl)-4-
     (trifluoromethyl) - (CA INDEX NAME)
/ Structure 80 in file .gra /
```

```
ACCESSION NUMBER:
                      2003:912358 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                       139:381381
TITLE:
                       Preparation of antibacterial pyridinedicarbonitriles
INVENTOR(S):
                       Grant, Richard; Latham, Christopher J.; Thomson,
                       Samantha; Zhao, Lihua
PATENT ASSIGNEE(S):
                       Pantherix Ltd., UK
SOURCE:
                       Brit. UK Pat. Appl., 18 pp.
                       CODEN: BAXXDU
DOCUMENT TYPE:
                       Patent
                       English
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                      KIND DATE
                                       APPLICATION NO.
    PATENT NO.
                                                             DATE
                                        ______
                             _____
    GB 2388593
                      A
                             20031119 GB 2002-10898
                                                              20020513
PRIORITY APPLN. INFO.:
                                        GB 2002-10898
                                                             20020513
                 MARPAT 139:381381
OTHER SOURCE(S):
GΙ
/ Structure 81 in file .gra /
AΒ
    The title compds. [I; n = 0-2; R1 = H, alkyl, CN, aryl, etc.] which have
    antibacterial activity, esp. against gram pos. ***bacteria*** , were
    prepd. Thus, reacting 2-amino-3,5-dicyano-6-mercaptopyridine with
    2-chloro-N-(2,5-dimethylphenyl)acetamide in the presence of K2CO3 in DMF
    afforded 19% I [n = 0; R1 = 2,5-Me2C6H3] which showed IC50 in the range of
    1-50 .mu.M against isolated Streptococcus pneumoniae chorismate synthase.
    Pharmaceutical compn. comprising the compd. I is claimed.
ΙT
      ***298216-30-5P***
                           ***303065-59-0P***
                                                 ***303065-61-4P***
      ***303065-63-6P***
                          ***311314-38-2P***
                                                ***311314-61-1P***
                          ***311789-13-6P***
                                                ***311795-13-8P***
      ***311332-03-3P***
                           ***312509-66-3P***
      ***312318-88-0P***
                                                 ***312513-87-4P***
                           ***318258-92-3P***
      ***312513-88-5P***
                                                 ***329206-96-4P***
                          ***331966-90-6P***
      ***331421-74-0P***
                                                 ***331966-91-7P***
                          ***332114-15-5P***
      ***331966-98-4P***
                                               ***337918-65-7P***
                           ***337926-03-1P*** , Acetamide, N, N'-(9H-fluoren-
      ***337918-66-8P***
9_
    ylidenedi-4,1-phenylene)bis[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-
      ***348146-19-0P***
                           ***348580-92-7P***
                                                 ***348581-11-3P***
      ***356589-29-2P***
                          ***356589-40-7P***
                                                ***356589-45-2P***
      ***356589-52-1P***
                          ***356589-54-3P***
                                               ***356589-62-3P***
      ***356589-71-4P***
                          ***400864-06-4P***
                                                ***625109-52-6P***
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
    (Uses)
       (prepn. of antibacterial pyridinedicarbonitriles)
RN
    298216-30-5 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-cyanophenyl)-
    (CA INDEX NAME)
```

L17 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

```
/ Structure 82 in file .gra /
     303065-59-0 CAPLUS
RN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2,6-
CN
     dimethylphenyl) - (CA INDEX NAME)
/ Structure 83 in file .gra /
RN
     303065-61-4 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-methylphenyl)-
     (CA INDEX NAME)
/ Structure 84 in file .gra /
RN
     303065-63-6 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3-methylphenyl)-
CN
     (CA INDEX NAME)
/ Structure 85 in file .gra /
RN
     311314-38-2 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-bromophenyl)-
     (CA INDEX NAME)
/ Structure 86 in file .gra /
     311314-61-1 CAPLUS
RN
    Acetamide, N, N'-(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)bis[2-[(6-amino-
     3,5-dicyano-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)
/ Structure 87 in file .gra /
     311332-03-3 CAPLUS
RN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3-methoxyphenyl)-
CN
     (CA INDEX NAME)
/ Structure 88 in file .gra /
RN
     311789-13-6 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N,N-diphenyl- (CA
CN
     INDEX NAME)
/ Structure 89 in file .gra /
     311795-13-8 CAPLUS
RN
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[3-
     (trifluoromethyl)phenyl]- (CA INDEX NAME)
```

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/ Structure 90 in file .gra /
     312318-88-0 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-butoxyphenyl)-
CN
     (CA INDEX NAME)
/ Structure 91 in file .gra /
RN
     312509-66-3 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2,5-
     dimethylphenyl) - (CA INDEX NAME)
/ Structure 92 in file .gra /
RN
     312513-87-4 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-ethoxyphenyl)-
     (CA INDEX NAME)
/ Structure 93 in file .gra /
     312513-88-5 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-ethoxyphenyl)-
CN
     (CA INDEX NAME)
/ Structure 94 in file .gra /
     318258-92-3 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-phenyl- (CA INDEX
CN
    NAME)
/ Structure 95 in file .gra /
     329206-96-4 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-bromophenyl)-
CN
     (CA INDEX NAME)
/ Structure 96 in file .gra /
RN
     331421-74-0 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-cyanophenyl)-
     (CA INDEX NAME)
/ Structure 97 in file .gra /
RN
     331966-90-6 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-methoxyphenyl)-
     (CA INDEX NAME)
/ Structure 98 in file .gra /
```

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RN
     331966-91-7 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-methoxyphenyl)-
     (CA INDEX NAME)
/ Structure 99 in file .gra /
     331966-98-4 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2-fluorophenyl)-
     (CA INDEX NAME)
/ Structure 100 in file .gra /
     332114-15-5 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[4-
     (aminosulfonyl)phenyl]- (CA INDEX NAME)
/ Structure 101 in file .gra /
     337918-65-7 CAPLUS
RN
    Acetamide, N,N'-1,4-phenylenebis[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-
       (CA INDEX NAME)
/ Structure 102 in file .gra /
RN
     337918-66-8 CAPLUS
     Acetamide, N,N'-(2-chloro-1,4-phenylene)bis[2-[(6-amino-3,5-dicyano-2-
     pyridinyl)thio] - (CA INDEX NAME)
/ Structure 103 in file .gra /
     337926-03-1 CAPLUS
RN
     Acetamide, N,N'-(9H-fluoren-9-ylidenedi-4,1-phenylene)bis[2-[(6-amino-3,5-
CN
     dicyano-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)
/ Structure 104 in file .gra /
RN
     339153-44-5 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-chlorophenyl)-
     (CA INDEX NAME)
/ Structure 105 in file .gra /
     339576-16-8 CAPLUS
RN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-methylphenyl)-
     (CA INDEX NAME)
/ Structure 106 in file .gra /
```

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RN
     339584-40-6 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(4-methoxy-2-
CN
     nitrophenyl) - (CA INDEX NAME)
/ Structure 107 in file .gra /
RN
     348146-19-0 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-[4-[(2-amino-3,5-dicyano-2-pyridiny1)thio]]
     thiazolylamino)sulfonyl]phenyl]- (CA INDEX NAME)
/ Structure 108 in file .gra /
RN
     348580-92-7 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3,4-
CN
     dichlorophenyl) - (CA INDEX NAME)
/ Structure 109 in file .gra /
     348581-11-3 CAPLUS
RN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2,6-
CN
     dichlorophenyl) - (CA INDEX NAME)
/ Structure 110 in file .gra /
RN
     356589-29-2 CAPLUS
     Acetamide, N-[4-(acetylamino)phenyl]-2-[(6-amino-3,5-dicyano-2-
CN
     pyridinyl)thio]- (CA INDEX NAME)
/ Structure 111 in file .gra /
     356589-40-7 CAPLUS
RN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[4-
CN
     (methylthio)phenyl]- (CA INDEX NAME)
/ Structure 112 in file .gra /
     356589-45-2 CAPLUS
RN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(9,10-dihydro-9,10-
CN
     dioxo-2-anthracenyl) - (CA INDEX NAME)
/ Structure 113 in file .gra /
     356589-52-1 CAPLUS
RN
     Benzoic acid, 4-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-
CN
     (CA INDEX NAME)
/ Structure 114 in file .gra /
RN
    356589-54-3 CAPLUS
```

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CN
     Benzoic acid, 3-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-
     (CA INDEX NAME)
/ Structure 115 in file .gra /
     356589-62-3 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[2-chloro-5-
     (trifluoromethyl)phenyl]- (CA INDEX NAME)
/ Structure 116 in file .gra /
     356589-71-4 CAPLUS
CN
     Benzoic acid, 5-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-2-
     chloro- (CA INDEX NAME)
/ Structure 117 in file .gra /
     400864-06-4 CAPLUS
RN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-2-naphthalenyl-
CN
     (CA INDEX NAME)
/ Structure 118 in file .gra /
     625109-52-6 CAPLUS
RN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3,4-
CN
     dimethylphenyl) - (CA INDEX NAME)
/ Structure 119 in file .gra /
       ***111971-56-3***
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of antibacterial pyridinedicarbonitriles)
RN
     111971-56-3 CAPLUS
     3,5-Pyridinedicarbonitrile, 6-amino-1,2-dihydro-2-thioxo- (CA INDEX NAME)
CN
/ Structure 120 in file .gra /
REFERENCE COUNT:
                               THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2003:145365 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         139:270296
TITLE:
                         Novel 4-aminopyrimido[4,5-b]quinoline derivatives as
                         potential antimicrobial agents
AUTHOR(S):
                         El-Sayed, Ola A.; El-Bieh, Fatma M.; El-Aqeel, Shada
                         I.; Al-Bassam, Badr A.; Hussein, Maher E.
CORPORATE SOURCE:
                         Pharmaceutical Chemistry Department, Faculty of
                         Pharmacy, University of Alexandria, Alexandria, 21521,
                         Egypt
SOURCE:
                         Bollettino Chimico Farmaceutico (2002), 141(6),
```

461-465

CODEN: BCFAAI; ISSN: 0006-6648

PUBLISHER: Societa Editoriale Farmaceutica

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

/ Structure 121 in file .gra /

AB Two series of 4-aminopyrimido[4,5-b]quinoline derivs. substituted in the 2-position, e.g. I, and/or in 1-position, e.g. II, have been prepd. by facile routes starting from 2-amino-3-cyanoquinoline 2,2-chloro-3-cyanoquinoline, and 2-arylamino-3-cyanoquinolines. The reactions involved simple fusion with thiourea or urea and, in some cases, with guanidine. The prepd. compds. were in vitro tested for antimicrobial activities against some selected Gram-pos., Gram-neg. \*\*\*bacteria\*\*\* and fungi. Products contg. the thio-function were the most active followed by those contg. the imino-function while the carbonyl contg. derivs. were without significant antimicrobial effect.

IT \*\*\*69513-35-5P\*\*\*

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of)

RN 69513-35-5 CAPLUS

CN 3-Quinolinecarbonitrile, 1,2-dihydro-2-thioxo- (CA INDEX NAME)

/ Structure 122 in file .gra /

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:221628 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 130:325083

TITLE: Synthesis and antimicrobial activity of some new

4-methylquinolines

AUTHOR(S): Kamel, M. M.; Fathala, O. A.; Abdou, W. A. M.; Haiba,

М. Е.

CORPORATE SOURCE: Medicinal Chemistry Department, National Research

Centre, Cairo, Egypt

SOURCE: Proceedings of the Pakistan Academy of Sciences

(1997), 34(1), 7-11

CODEN: PKSPAW; ISSN: 0377-2969 Pakistan Academy of Sciences

DOCUMENT TYPE: Journal LANGUAGE: English

PUBLISHER:

AB Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridine-6-yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinoline Mannich bases were synthesized for the purpose of antimicrobial evaluation against \*\*\*bacteria\*\*\* , yeast, and fungi. Two compds. showed activity

against these microorganisms.

IT \*\*\*218272-67-4P\*\*\* \*\*\*218272-68-5P\*\*\* \*\*\*218272-69-6P\*\*\*

\*\*\*218272-70-9P\*\*\* \*\*\*223697-02-7P\*\*\*

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

```
BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of methylquinolines as antibacterial and antifungal agents)
RN
     218272-67-4 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
CN
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 123 in file .gra /
RN
     218272-68-5 CAPLUS
     CN
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 124 in file .gra /
RN
     218272-69-6 CAPLUS
CN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
    dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 125 in file .gra /
     218272-70-9 CAPLUS
CN
     3-Pyridine carbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
    dihydro-4-(2-thienyl)-2-thioxo- (CA INDEX NAME)
/ Structure 126 in file .gra /
     223697-02-7 CAPLUS
    3-Pyridinecarbonitrile, 6-[4-[(7-chloro-4-methyl-2-
CN
    quinolinyl)amino]phenyl]-1,2-dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA
     INDEX NAME)
/ Structure 127 in file .gra /
REFERENCE COUNT:
                        17
                              THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
                              RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
                        1998:702455 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        130:66375
TITLE:
                        Synthesis of some new 4-methylquinolines of possible
                        biological activity
                        Kamel, M. M.; Fathalla, O. A.; Abdou, W. A. M.; Omer,
AUTHOR(S):
                        M. T.; Haiba, M. E.
CORPORATE SOURCE:
                        Medicinal Chemistry Department, National Research
                        Centre, Cairo, Egypt
SOURCE:
                        Egyptian Journal of Pharmaceutical Sciences (1998),
                        Volume Date 1997, 38(1-3), 79-86
                        CODEN: EJPSBZ; ISSN: 0301-5068
PUBLISHER:
                        National Information and Documentation Centre
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        English
    Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridin-6-
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yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinolines
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
             ***bacteria*** , yeast, and fungi. 7-Chloro-4-methyl-2-[4-
     hydroxy-3,5-di(diethylaminomethyl) anilinoquinoline showed fungicidal
     activity against Aspergillus niger.
       ***218272-67-4P***
                             ***218272-68-5P***
                                                    ***218272-69-6P***
ΤT
       ***218272-70-9P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis and antimicrobial activity of 4-methylquinolines)
RN
     218272-67-4 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
CN
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 128 in file .gra /
RN
     218272-68-5 CAPLUS
CN
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 129 in file .gra /
     218272-69-6 CAPLUS
CN
     3-Pyridine carbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 130 in file .gra /
     218272-70-9 CAPLUS
     3-Pyridine carbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
CN
     dihydro-4-(2-thienyl)-2-thioxo- (CA INDEX NAME)
/ Structure 131 in file .gra /
REFERENCE COUNT:
                               THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
                         15
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1998:702449 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         130:81446
                         Synthesis of some new indole derivatives of possible
TITLE:
                         antimicrobial activity
AUTHOR(S):
                         Fahmy, H. H.; Kassem, E. M. M.; Abdou, W. A. M.;
                         Mahmoud, S. A.
CORPORATE SOURCE:
                         Department of Medicinal Chemistry, National Research
                         Centre, Cairo, Egypt
                         Egyptian Journal of Pharmaceutical Sciences (1998),
SOURCE:
                         Volume Date 1997, 38(1-3), 13-22
                         CODEN: EJPSBZ; ISSN: 0301-5068
                         National Information and Documentation Centre
PUBLISHER:
DOCUMENT TYPE:
                         Journal
                         English
AΒ
     A series of indolyl arylidene hydrazones, indolylamidothiazolidin-4-ones,
     pyrazoline and pyrazolidindione derivs., 3-(3-cyano-4-aryl-2-imino-(1H)-
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pyridin-6-yl)-indoles and 3-(3-cyano-4-aryl-2-thioxo-(1H)-pyridin-6-yl)-
     indoles were synthesized. Some of the new compds. showed considerable
     antimicrobial activity against gram + ve ***bacteria*** , yeast and
     fungi.
       ***218784-55-5P***
                              ***218784-56-6P***
                                                     ***218784-57-7P***
ΤТ
       ***218784-58-8P***
                              ***218784-59-9P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (synthesis of new indole derivs. of possible antimicrobial activity)
RN
     218784-55-5 CAPLUS
CN
     3-Pyridinecarbonitrile, 1,2-dihydro-6-(1H-indol-3-yl)-4-phenyl-2-thioxo-
     (CA INDEX NAME)
/ Structure 132 in file .gra /
     218784-56-6 CAPLUS
     3-Pyridinecarbonitrile, 1,2-dihydro-6-(1H-indol-3-yl)-4-(4-methoxyphenyl)-
CN
     2-thioxo- (CA INDEX NAME)
/ Structure 133 in file .gra /
RN
     218784-57-7 CAPLUS
     3-Pyridinecarbonitrile, 4-(4-chlorophenyl)-1,2-dihydro-6-(1H-indol-3-yl)-2-
CN
     thioxo- (CA INDEX NAME)
/ Structure 134 in file .gra /
     218784-58-8 CAPLUS
RM
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-1,2-dihydro-6-(1H-
CN
     indol-3-yl)-2-thioxo- (CA INDEX NAME)
/ Structure 135 in file .gra /
     218784-59-9 CAPLUS
RN
     3-Pyridine carbonitrile, 1,2-dihydro-6-(1H-indol-3-yl)-2-thioxo-4-(3,4,5-
CN
     trimethoxyphenyl) - (CA INDEX NAME)
/ Structure 136 in file .gra /
REFERENCE COUNT:
                         16
                               THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
                         1994:134144 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         120:134144
ORIGINAL REFERENCE NO.: 120:23615a,23618a
TITLE:
                        Preparation of cephalosporin derivatives as
                         antibacterial agents
INVENTOR(S):
                         Tanaka, Kyoshi; Sutani, Mineichi; Komatsu, Miwako;
                         Tsuchida, Keiichi; Saito, Akito; Hayashi, Kazuya;
                         Kanna, Hiroshi; Yonezawa, Kenji; Minami, Shinzaburo;
```

Watanabe, Yasuo

PATENT ASSIGNEE(S): Toyama Chemical Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 26 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05202065	А	19930810	JP 1991-311552	19911031
JP 05262777	A	19931012	JP 1991-343936	19911202
JP 3141041	B2	20010305		
PRIORITY APPLN. INFO.:			JP 1991-311552	A1 19911031
OTHER SOURCE(S):	MARPAT	120:134144		
GI				

/ Structure 137 in file .gra /

The title .beta.-lactams [I; R1 = (un)protected NH2; R2 = (cyano-, AΒ carbamoyl-, or halo-substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; R3 = (un)protected CO2H, CO2-; R4 = H, (un)protected NH2; A = CH, CX; X = halo; B = bond, CH2NH, alkylene or O-lower alkylene optionally substituted with (un)protected hydroxy; D = NR5R6; R5 = H, H2N-protecting group; R6 = H, (cyano-, carbamoyl-, or halo-substituted) alkyl, alkenyl, aryl, or cycloalkyl; B-D = (halo)alkoxy; n = 0,1], having potent antibacterialactivity against gram pos. \*\*\*bacteria\*\*\* including methicillin-resistant Staphylococcus aureus strains, are prepd. Thus, quaternization of 3-tert-butoxylcarbonylaminothieno[2,3-b]pyridine by p-methoxybenzyl 3-iodomethyl-7-[(Z)-2-methoxyimino-2-(2-tritylaminothiazol-4-yl)acetamido]-3-cephem-4-carboxylate in DMF at room temp. followed by deprotection with CF3CO2H in anisole gave 7-[2-(2-aminothiazol-4-yl)-(Z)-2methoxyiminoacetamido]-3-(3-amino-7-thieno[2,3-b]pyridinio)methyl-3-cephem-4-carboxylate (II). II showed min. inhibitory concn. of 1.56, 12.5, .ltoreq.0.1, and 1.56 .mu.g/mL against .beta.-lactamase-producing Staphylococcus aureus F-137, methicillin-resistant S. aureus F-597, Escherichia coli NIHJ JC-2, and Pseudomonas aeruginosa IFO 3445, resp. A total of 32 I were prepd.

\*\*\*152939-12-3P\*\*\* \*\*\*152939-11-2P\*\*\* ΤT

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of, as intermediate for antibacterial cephalosporin deriv.)

RN 152939-11-2 CAPLUS

CN Acetic acid, 2-[(3-cyano-5-nitro-2-pyridinyl)thio]-, methyl ester (CA INDEX NAME)

/ Structure 138 in file .gra /

RN 152939-12-3 CAPLUS

CN Acetic acid, 2-[(5-amino-3-cyano-2-pyridinyl)thio]-, methyl ester (CA INDEX NAME)

/ Structure 139 in file .gra /

L17 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:514821 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 105:114821

ORIGINAL REFERENCE NO.: 105:18579a,18582a

TITLE: 2-(2-Aminothiazol-4-yl)-2-alkoxyiminoacetic acid

derivatives substituted on the oxime

INVENTOR(S): Heymes, Rene; Vignau, Michel

PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.

SOURCE: Fr. Demande, 66 pp. Addn. to Fr. Demande Appl. No. 78

09617.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
FR 2553770	A2	19850426	FR 1983-16698		19831020
FR 2553770	В2	19860314			
FR 2438050	A2	19800430	FR 1978-24563		19780824
FR 2438050	B2	19830415			
AT 8100043	A	19821115	AT 1981-43		19810108
AT 371472	В	19830627			
US 4439433	A	19840327	US 1981-267638		19810527
GB 2101117	A	19830112	GB 1981-34540		19811117
GB 2101117	В	19830602			
CH 642648	A5	19840430	CH 1983-1949		19830411
PRIORITY APPLN. INFO.:			FR 1978-24563		19780824
			FR 1978-9617	A	19780331
			AT 1979-2403	A	19790330
			CH 1979-3008	A	19790330
			GB 1979-11275	A	19790330
			US 1979-25666	А3	19790330

OTHER SOURCE(S): CASREACT 105:114821; MARPAT 105:114821

GΙ

/ Structure 140 in file .gra /

2-(2-Aminothiazol-4-yl)-2-alkoxyiminoacetic acid derivs. I [R = CXR2 (X = O, S; R2 = alkyl, alkoxy, Ph, substituted amino, substituted carboxyl, etc.,); R1 = Cl, OMe, alkyl, cycloalkyl, alkylthio, acetoxymethyl, carbamoyloxymethyl, etc.; A = H, alk. metal, alk. earth metal, etc.], having good activity against gram-pos. \*\*\*bacteria\*\*\* (for example, the MIC for penicillin-resistant Staphylococcus was 1 .mu.g/mL after 24 and 48 h), are prepd. Thus, syn-2-[(2-bromoethoxy)imino]-2-(2-tritylaminothiazol-4-yl)acetic acid [prepd. in 2 steps from Et 2-hydroxyimino-2-(2-tritylamino-4-thiazolyl)acetate-HCl] was acylated with tert-Bu 7-aminocephalosporanate to give tert-Bu 3-acetoxymethyl-7-[[2-(2-tritylaminothiazol-4-yl)-2-[2-bromoethoxy)imino]acetyl]amino]ceph-3-em-4-carboxylate (II). II was then deprotected and converted to the trifluoroacetate of syn-3-acetoxymethyl-7-[[2-(2-aminothiazol-4-yl)-2-[(2-bromoethoxy)imino]acetyl]amino]ceph-3-em-4-carboxylic acid.

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***72697-85-9P***
TT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and deblocking of)
RN
     72697-85-9 CAPLUS
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     3-[(acetyloxy)methyl]-7-[[[[2-[(3-cyano-6-methyl-2-
     pyridinyl)thio]ethoxy]imino][2-[(triphenylmethyl)amino]-4-
     thiazolyl]acetyl]amino]-8-oxo-, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA
     INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 141 in file .gra /
ΙT
       ***72697-31-5P***
                            ***72697-32-6P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (prepn. of, as antibiotic)
     72697-31-5 CAPLUS
RN
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     3-[(acetyloxy)methyl]-7-[[(2-amino-4-thiazolyl)[[2-[(3-cyano-6-methyl-2-
     pyridinyl)thio]ethoxy]imino]acetyl]amino]-8-oxo-, [6R-
     [6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 142 in file .gra /
    72697-32-6 CAPLUS
RN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     3-[(acetyloxy)methyl]-7-[[(2-amino-4-thiazolyl)[[2-[(3-cyano-6-methyl-2-
     pyridinyl)thio]ethoxy]imino]acetyl]amino]-8-oxo-, monosodium salt,
     [6R-[6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 143 in file .gra /
=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
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COST IN U.S. DOLLARS
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                                                      ENTRY
                                                              SESSION
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                                                                 -15.20
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